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Aerospace and Materials Sciences Directorate
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CHARACTERIZATION OF DISLOCATION CORE STRUCTURES IN BCC METALS

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I. EXECUTIVE SUMMARY

The scientific aim of this study was to use state-of-the-art TEM techniques to experimentally describe dislocation core structures in bcc metals through experimental characterization of screw dislocations in single-crystalline Mo. Methods were developed for deriving localized electron structure data from electron energy loss spectra (EELS) taken from perfect lattice regions and along dislocations and low angle boundaries in ordered NiAl. Significant changes in the fine structure of the Ni $L_{2,3}$ edge were associated with <001> dislocations in NiAl and comparisons with first-principles were used to characterize localized electronic structure and bonding in the vicinity of this dislocation. However, difficulties associated with the position of the energy edges for Mo precluded application of this technique to the study of ½<111> screw dislocations in single-crystalline Mo. For this reason, the majority of this study focused on: direct HREM observations of the atomic columns surrounding ½<111> screw dislocations in Mo, characterization of the displacement fields associated with these dislocations, mitigation of experimental noise, and comparison of the experimental observations with theoretically predicted dislocation structures. Direct displacement plots of the HREM images revealed an apparent three-fold symmetry of the Mo screw dislocation similar to what was previously reported by Sigle [1], but comparison with image simulations indicated that this result was entirely misleading. Closer inspection of the images indicated that atomic displacements associated with the "Eshelby Twist" (free surface relaxations) masked the core displacements and precluded direct comparison with core predictions based on atomistic and first-principles analysis. Nye tensor analysis, as conducted in collaboration with Dr. Hartley and Professor Mishin, proved to be highly effective in removing the Eshelby Twist. Although the Eshelby twist was removed from the experimental HREM images some residual, mottled contrast structure was observed in the Nye tensor plots. This contrast was found to be due to experimental noise, which masks the true structure of the dislocation core and precludes detailed characterization of screw dislocations in Mo by HREM.

II. RESEARCH OBJECTIVES

The overarching objective of the current study was to explore the techniques necessary for providing quantitative measurements of dislocation core structures in bcc metals and alloys that can be used provide benchmarks for theoretical models and allow us to better understand the role that dislocation core structure plays in determining the dislocation mobility and strength of bcc metals and alloys. Important differences in the atomic structure of stressed and unstressed dislocation cores in group VB and VIB bcc metals have been predicted [2,3], and one of the primary goals of this study is to provide experimental observations with which to compare these predictions. Experimental HREM images, simulated HREM images (based on anisotropic elasticity, atomistic and *ab initio* predictions of the core geometry), and various methodologies for describing the spatial distribution of atomic displacement in the dislocated crystal (direct displacement, differential displacement, Fourier filtering, and Nye tensor analysis) were compared and contrasted in an effort to characterize the near core region of a/2<111> screw dislocations in ultra-pure Mo single crystals.

III. TECHNICAL ACCOMPLISHMENTS

III A. Electronic structures of dislocations and small angle boundaries

First-principles calculations have been used to predict the electronic structure of the atoms in and around the core of a dislocation, which naturally allow for a better description of the core structure. In addition, knowledge of the electronic structure of the dislocation core will benefit the understanding of the influence of dislocations upon the physical and mechanical properties of materials. The local electronic structure of a material can be experimentally determined from electron energy-loss spectrum (EELS) of an electron beam scattered through it. However, it is a non-trivial challenge to develop modern electron microscope technique for acquiring an electron energy-loss spectrum at a dislocation core because of the requirements for high intensity, extremely small beam size, and slow sample drift at extremely high magnification. Recently, several successes have been achieved in semiconductor materials by using VG STEM [4,5], but no results have been reported on the use of EELS to characterize the electronic structure of dislocations in metallic materials with commercial transmission electron microscopes (CTEM).

In this study, the characterization of the electronic structure of dislocation cores and grain boundaries was conducted by employing a Phillips CM-300 FEG in nano-probe mode. We first determined that the energy resolution depends on the electron beam coherence rather than the beam size and that parallel illumination with a nano- or subnano- size yields a higher energy resolution than a convergent beam. Thus, using nano-probe mode a difference in the spectra of defects (grain boundaries and dislocations) and perfect crystal regions could be measured, see for example Fig. 1, which demonstrates the fact that CTEM has the capability to probe the local electronic structure of these defects.

The example given in this figure shows that significant changes in the fine structure of the Ni $L_{2,3}$ edge spectra taken at and away from the dislocation core can be observed. The effect of beam damage is excluded by the fact that the change in fine structure is only observed when the beam is positioned on the dislocation. The splitting of the $L_{2,3}$ edge and the increase in absorption is most likely due to the "broken bonds" in the core as suggested by first principle calculations [6]. Correct interpretation of the relation between localized electronic bonding and the fine structure in the EELS spectra will require simulations based on first-principles calculations and were beyond the scope of the current program. Attempts at characterizing of the electronic structure of dislocation cores and grain boundaries in bcc Mo was attempted but precluded by the unfavorable location of the energy loss edges for Mo.

III B. Atomic structure of dislocation cores in bcc molybdenum

Differences in the predications of atomistic and the first-principles calculations point to the need for comparison with experimental observations, but the difficulties associated with the compact nature of these cores and the fact that edge components of these dissociated screw dislocations are extremely small make experimental characterization and interpretation of the core structures an extremely difficult task. At the start of this project, only one limited HRTEM observations of the screw dislocations in a bcc metal had been reported [1].

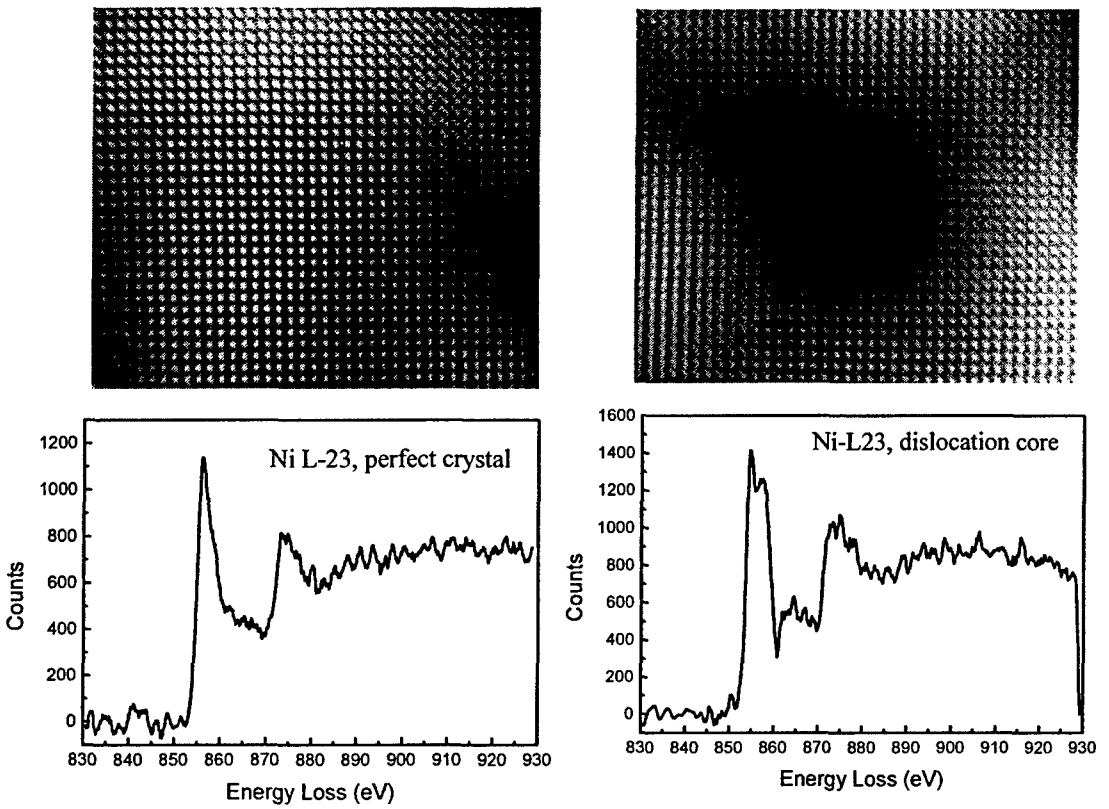
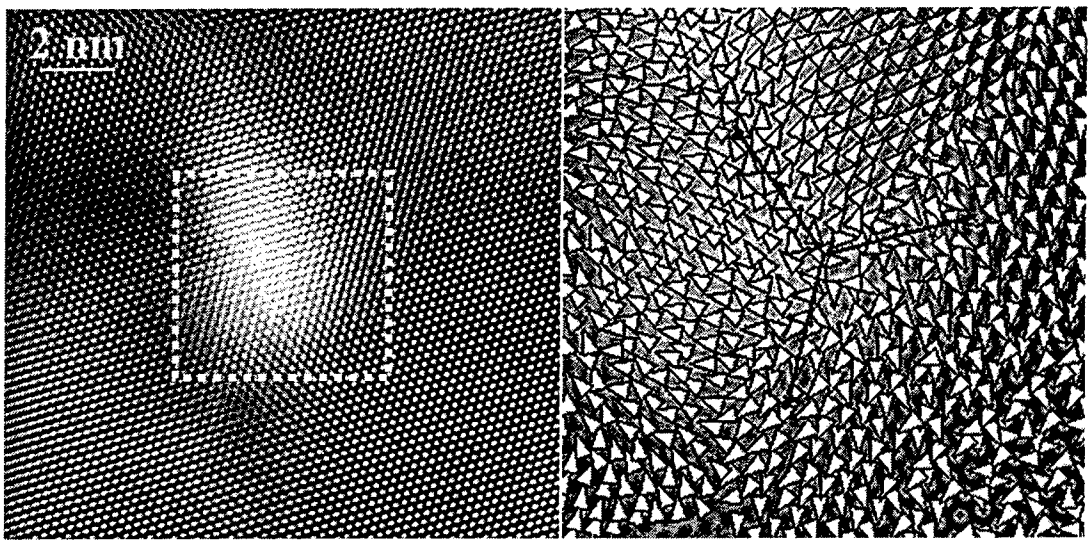


Fig. 1: HREM images and electron energy loss spectra of Ni $L_{2,3}$ edge measured by using a nano-probe with a beam size of 1.2 nm, (a) from a perfect crystal region; and (b) from the core region of a <100> edge dislocation in B2 NiAl.

In HREM, screw dislocations are aligned end-on, i.e. parallel to the thickness of the TEM foil. Hence only the edge displacements can be detected (the screw displacements are not observed since they are perpendicular to the viewing plane). The <111> bcc projection is also a convenient zone axis for HREM since the {110} interplanar spacing is approximately 2.2 Å for molybdenum, which is within the point resolution of most microscopes. This is not the case, however, for Mo edge dislocations on {110} planes parallel to <112>. A typical <112> bcc HREM image consists of lattice fringes rather than fully resolved atom column positions.

Our investigation of the atomic structure of a/2<111> screw dislocations in bcc metals was started by preparing dislocation containing and <111> oriented TEM foils of single-crystalline Mo. Fig. 2(a) shows an HRTEM micrograph of a screw dislocation, taken with a defocus of –72 nm. Although the bright and dark contrast generated by the elastic strain field of the dislocation can be seen, the core is very compact and the in-plane displacements around the dislocation cannot be directly identified from the atomic resolution image by eye. In an attempt to measure the dissociation of the dislocation and to display visual determination of the exact location of the core, an NCEM software package was employed to

determine the in-plane displacements of atomic column positions in the HRTEM micrograph, that are caused by the presence of the dissociated dislocation. The preliminary results (Fig. 2(b)) suggest that displacements around the core exhibit a quasi three-fold symmetry similar to that reported by Sigle [1]. It is however important to note that the magnitudes of the displacements in this direct displacement plot are masked by the arrowheads drawn by the NCEM software. To address this shortcoming we subsequently experimented with several techniques that we hoped would allow us to quantify the in-plane displacements in the HREM image in a way that would allow for more direct comparisons with theoretical predications of the atomic structure.



(a) (b)

Fig. 2: (a) HRTEM micrograph of $^{a}/_{2}$<111> screw dislocation in a single crystal Mo; and (b) the displacement map of the core determined by the NCEM software package.

Phase Image Analysis. The continuous displacement fields around dislocations obtained in this study were then measured by the software, *NCEM Phase Extensions*, which was developed by Drs. Kilaas and Hytch to analyze of variations in structure from high-resolution electron microscope (HREM) images by combining real space and Fourier information [3,4]. The HREM contrast or intensity distribution (*I(r)*) of dislocations that is produced by the displacement around the defects can be described as

$$I(r) = \sum I_0(r) e^{-2\pi i g.u(r)} e^{2\pi i g.r},$$

where **g** is the reciprocal lattice vectors describing the perfect lattice; and u(r) is displacement field caused by dislocations. By measuring two phase images, the two-dimensional displacement field can be determined by:

$$u(r) = [u(r_1).g_1.a_1 - u(r_2).g_2.a_2],$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the basis vectors for the lattice in real space corresponding to the reciprocal lattice defined by $\mathbf{g}_1$ and $\mathbf{g}_2$.

Hytch and colleagues have used this technique to measure the displacements around an edge dislocation in silicon and reported that the agreement of their observations with anisotropic elastic theory calculations was better than 0.003 nm [7]. In the current study, the displacement fields of two experimentally imaged dislocations were characterized by this method. The first is our previously published observation of a 60° dislocation in single crystalline iridium [8] and the second is a more recently obtained image of a <111> screw dislocation in molybdenum. The initial study being restricted to edge dislocations, the use of the geometric phase technique on these other two dislocations was undertaken in an attempt to explore the types of dislocations that can be characterized with this technique.

Figure 3(a) shows an HREM image of a 60° dislocation in single crystalline iridium. The Fourier Transform (FT) and the Power Spectrum (PS) calculated from the HREM image is shown in Fig. 3(b). By filtering in Fourier space, the inverse FT images corresponding to $\boldsymbol{g_1}$ and $\boldsymbol{g_2}$ in Fig. 3(b) are obtained, showing the visible and invisible conditions for the dislocation (Figs. 3(c,d). Actually, the discontinuous displacement around the core of the dislocation can be directly identified from the marked box in Fig. 3(c). The core of the dislocation spreads about seven lattice planes (1.1 nm), which is in good agreement with previously reported value (1.2 nm) that was determined by sequential matching of image simulations with the experimental image. After calculating the phase images of $\boldsymbol{g_1}$ and $\boldsymbol{g_2}$, the displacement field along the X and Y axes are presented in Figs. 3(e,f). Bright and dark contrast illustrates the magnitude of the displacement and the discontinuous characteristics of the displacement fields can be clearly recognized from the geometric phase analysis. The fact that the phase increases monotonically around the dislocation with abrupt transition from light to dark at the point (2π) where the phase is renormalized is similar to what has been reported for edge dislocations, but the plot itself is hard to interpret.

Unlike the 60° dislocations in fcc crystals and edge dislocations in cubic Si, no discontinuous displacement fields where found around the screw dislocation in bcc Mo. Although the HREM image (Fig. 4(a)) does show bright/dark contrast around the screw dislocation core, no clear displacement can be identified from the HREM micrograph and the filtered FT images (Fig. 4(c,d)). It is also important to note that this technique was found to be exceedingly sensitive to the input parameters and did not therefore have a satisfactory degree of reproducibility. For these reasons it was abandoned as a viable technique for characterizing screw dislocations in bcc Mo.

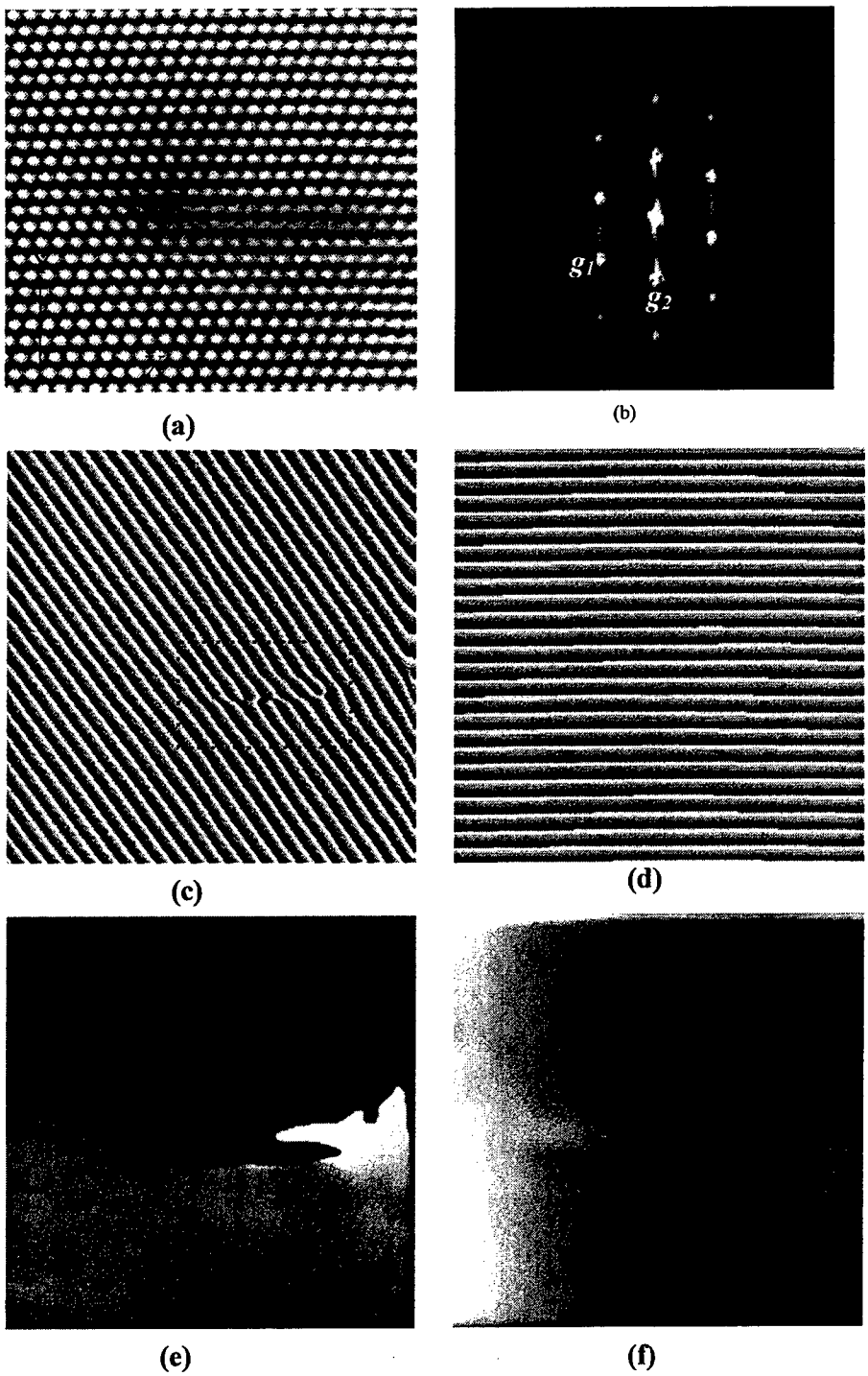


Fig. 3: Geometric phase analysis of an 60° dislocation in single crystal Ir. (a) HREM image; (b) FT &PS pattern; (c) Inverse FT image of g_1; (d) Inverse FT image of g_2; (e) Displacement map of U_x; and (f) Displacement map of U_y

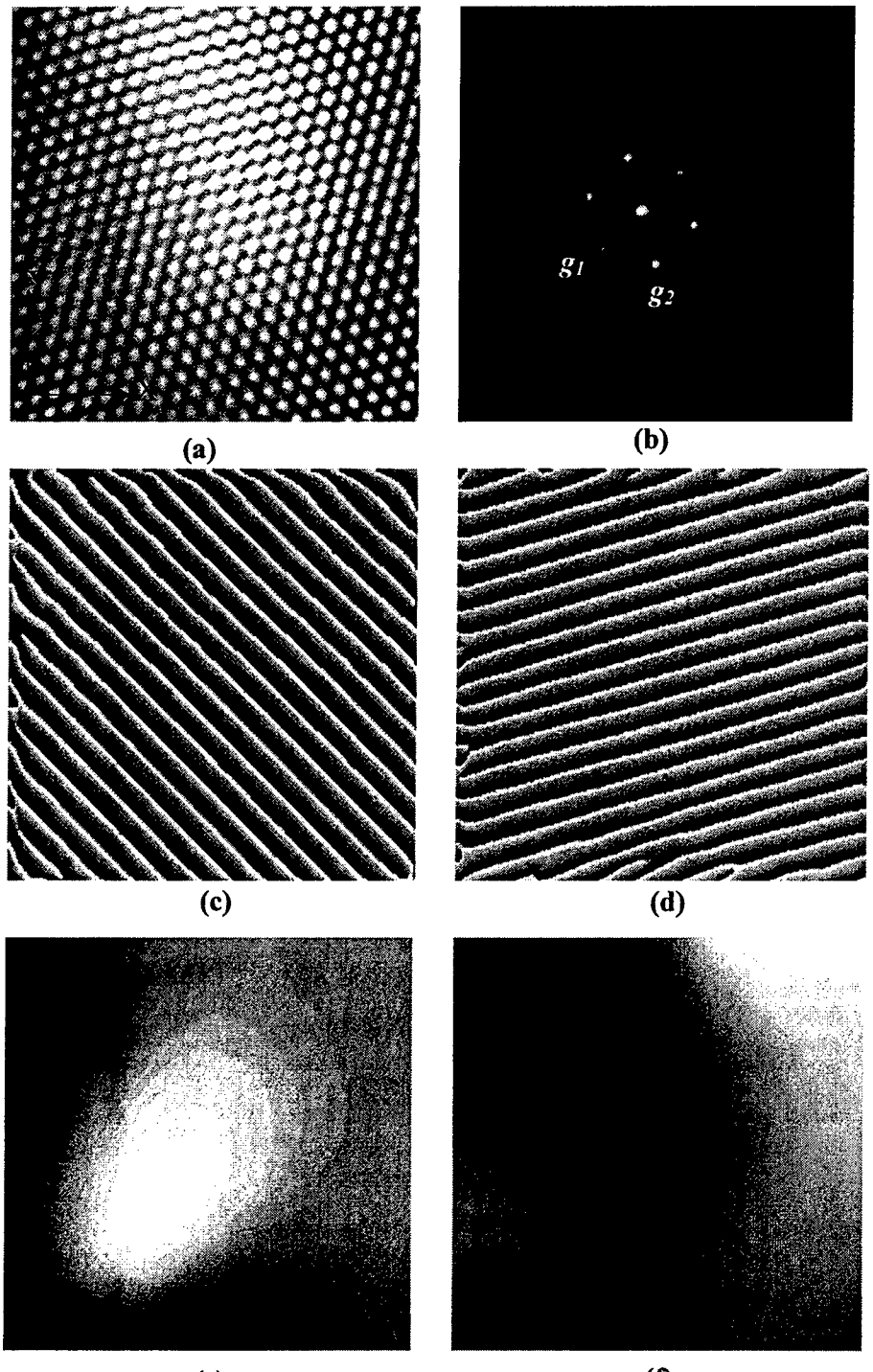


Fig. 4: Geometric phase analysis of a screw dislocation in bcc molybdenum. (a) HREM image; (b) FT &PS pattern; (c) Inverse FT image of g_1; (d) Inverse FT image of g_2; (e) Displacement map of U_x; and (f) Displacement map of U_y

Nye tensor analysis. The Nye tensor method [9], which maps the density of the components of the infinitesimal dislocation distribution in the near core region, was also investigated as a possible alternative. The theory for this technique and algorithm for calculating the Nye tensor have been presented in recent publications by Hartley and Mishin [10-12] and in the papers that we recently co-authored with them [13,14]. The Nye tensor technique has proven to be very effect and their assistance in implementing this analysis in the present study is gratefully acknowledged.

Figure 5 shows the Nye tensor plots for the first-principles dislocation core [3] calculated with a maximum angular distortion of 15°. The α_{33} plot (Fig. 5(a)) suggests that splitting of the dislocation into screw fractional dislocations does not take place. The edge fractional dislocations revealed by the α_{13} and α_{23} components (Figs. 5(b,c)) do, however, show some splitting although much less than is predicted by atomistic calculations [2] (to aid visualization Figs. 5(b), (c) and (d) are plotted on a scale of -0.005 $Å^{-1}$ to 0.005 $Å^{-1}$). Fig. 5(d) gives the Burgers vector magnitude of the edge fractional dislocations to reveal three fractional dislocations spread along {112} planes with Burgers vectors parallel to <112>. The A, B and C fractional dislocations in Fig. 5(d) all have a 0.01 Å (i.e. 0.005*b*) Burgers vector magnitude. A schematic of the dislocation splitting is given in fig. 5(e). This example illustrates the utility of the Nye tensor approach and gives an example of the level of detail and resolution that will be required in the experimental results.

Of significant importance in the observation of edge displacements in ½<111> screw dislocations is the inevitable presence of surface relaxation of the TEM foil. An end-on dislocation in a thin TEM foil is similar to a dislocation in a plate with parallel free surfaces. The finite thickness gives rise to elastic forces that axially twist the dislocation at the two free surfaces by equal and opposite amounts. This is the so-called Eshelby twist [15]. Since the individual atoms are subjected to only elastic forces the Eshelby twist is a compatible deformation. For compatible deformations the lattice correspondence tensor is equal to the gradient of a continuous deformation field. Hence the Nye tensor for compatible deformations (e.g. the Eshelby twist) is identically zero (cf. differential displacement plots which detect both compatible and incompatible deformations). For an end-on screw dislocation in a thin foil the Nye tensor should therefore be 'blind' to the surface relaxation but nevertheless detect the short range, incompatible deformation at the dislocation core region which is of interest to us.

Under appropriate HREM imaging conditions, an atom column is projected onto the plane of view as a single bright spot. Since the Eshelby twist is equal and opposite at the two free surfaces, the net displacement of an atom column integrated through the thickness of the TEM foil is zero. This does not however assure that the displacement of a projected atom column position, due to surface relaxation, is zero for an HREM image. An atom scatters the electron beam as a Huygen wavelet that spreads outwards (largely in the direction of the incident beam) until it is rescattered by other atoms in the crystal. A single electron will therefore undergo a series of scattering and propagation events before it leaves the TEM specimen. The overall scattering of the electrons results in HREM atom column displacements which do not represent the true deformation state of the Eshelby twist.

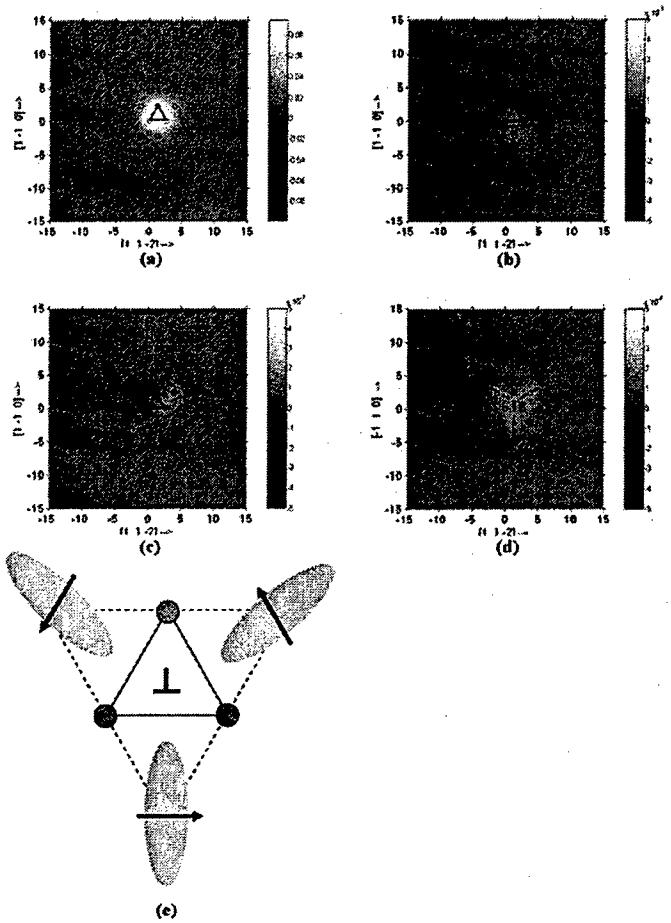


Fig. 5: Nye Tensor plots of (a) α_{33}, (b) α_{13} and (c) α_{23} components for the first-principles, ½<111> Mo screw dislocation. The dislocation is at the centre of the triangle outlined in each figure. For visualization α_{13} and α_{23} are plotted on a scale of -0.005 $Å^{-1}$ to 0.005 $Å^{-1}$. (d) plots the magnitude of the edge fractional dislocations. The {112} planes of spreading are as indicated by the dashed lines. A schematic of the dislocation splitting is shown in (e). The dislocation is at the position marked with the ⊥ symbol. The arrows give the orientation of the edge fractional dislocation Burgers vectors.

Figure 6 shows the results of an HREM image simulation performed using a supercell containing a screw dislocation with the Eshelby twist. In-plane displacements are observed for both the 5nm and 20nm thick foils although there is no shift in the averaged atom column positions. The displacement vectors in Figs. 6(a) and (b) were constructed by comparing projected atom column positions in the defect image to those in a simulated image of the perfect crystal. The displacement maps show circular symmetry, characteristic of the Eshelby twist. Surprisingly the displacements in the 20 nm foil are larger than that for the 5 nm specimen, despite the volume fraction of material undergoing surface relaxation being smaller for the former. The α_{13} and α_{23} Nye tensor plots (Figs. 6(c,d)) for the '2D crystal' given by the 5nm foil HREM image are featureless, indicating that even though the spots in the HREM image are displaced the overall 'deformation' is compatible in nature (note that the isotropic screw dislocation used in the simulations does not have any edge displacements). Similar Nye tensor results were obtained for the HREM image of the 20nm thick specimen, where the displacements are even greater (Fig. 6(b)).

Table 1 compares the HREM image Eshelby twist displacements observed in Figs. 6(a,b) and the edge displacements for a Mo screw dislocation in an infinite medium. The average and largest HREM image displacements were calculated for only the inner 110 atom columns (total number of atom columns is 182) since periodic boundary conditions affect the displacements for the outermost atom columns. The largest FS and BOP core displacements are smaller than the largest Eshelby twist displacements. It is therefore impossible to unambiguously determine the intrinsic edge displacements of a screw dislocation using direct displacement maps. However, the Nye tensor will eliminate any Eshelby twist displacements leaving only the incompatible edge displacements. This is of immense practical value since the use of thin foils in HREM makes surface relaxation unavoidable.

Table 1: Comparison of in-plane atomic displacements for the FS and BOP screw dislocation cores and the Eshelby twist observed in simulated HREM images.

In-plane displacements	**Magnitude (pm)**
Largest displacement (FS core)	7.8
Largest displacement (BOP core)	10.2
Largest Eshelby twist displacement (5 nm foil)	15.2
Average Eshelby twist displacement (5 nm foil)	11.5
Largest Eshelby twist displacement (20 nm foil)	40.8
Average Eshelby twist displacement (20 nm foil)	19.7

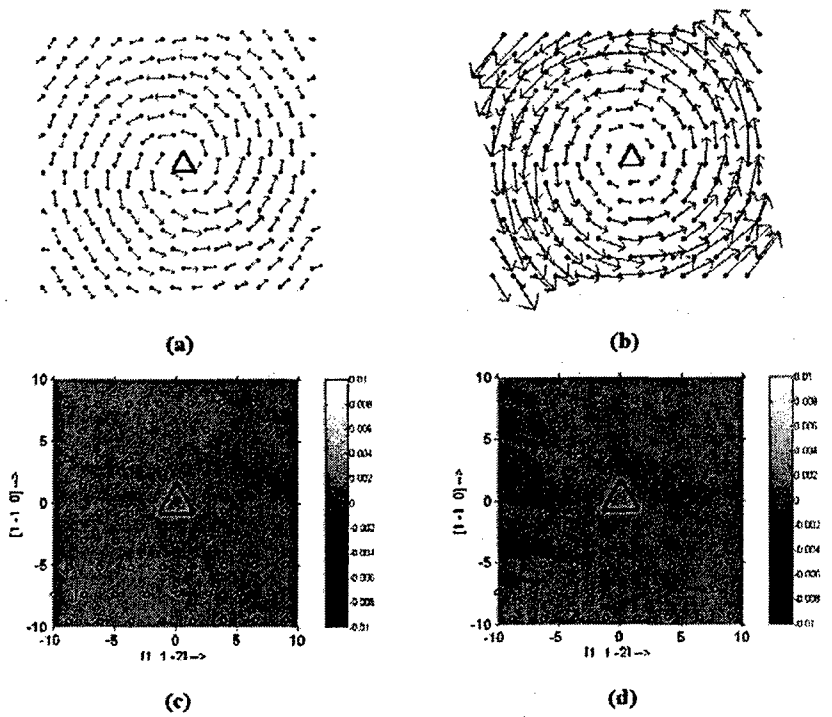


Fig. 6: Simulated HREM direct displacement maps for the (a) 5 nm and (b) 20 nm thick Mo foils containing the Eshelby twist. The vector magnification is x15. Nye tensor plots for the 5 nm foil HREM image are (c) α_{13} and (d) α_{23}. The screw dislocation is at the center of the triangle marked in each figure but the Nye plots do not pick up the Eshelby twist.

Figure 7 shows the α_{13} and α_{23} Nye tensor plots for a experimental HREM image of a screw dislocation in Mo. They were constructed by treating the centers of the bright spots in the image as individual 'atoms' that form a '2D crystal'. The Eshelby twist has been removed to within the background noise level. This clearly illustrates the value of the Nye tensor method in reducing unwanted contributions due to surface relaxation of a thin TEM foil. Edge displacements were not, however, detected in the dislocation core region, which is not surprising since the goodness of fit of the perfect lattice is nearly two pixels. In fact, the background noise level present in our experimental HREM micrographs prevents accurate determination of the extremely small edge fractional dislocations via the Nye tensor method.

To demonstrate this, atom column displacements present in an HREM micrograph of the perfect crystal were taken to represent the random error of the experiment (for an ideal experiment a perfect crystal should not give any displacements). The atom column displacements in an HREM image of a <111> oriented, perfect crystal region of bcc Mo was characterized by approximating the displacement magnitudes as a Gaussian distribution††; the orientation of the displacement vectors was found to be nearly uniformly distributed within the $[0\ 2\ \pi]$ radian interval. This background noise in the atomic displacements was then superimposed on the 2D projected, dislocated crystals of the FS, BOP and first-principles screw dislocation cores by using a Gaussian distributed random number generator for the displacement magnitude and a linear random number generator for the displacement orientation. The α_{13} and α_{23} Nye tensor plots for these modified supercells, e.g. Figs. 8(a,b), no longer showed the edge fractional dislocations apparent in figures 2, 4 and 5 respectively, but rather a characteristic mottled contrast structure. Close examination of the Nye tensor plots in Fig. 7 showed that this contrast is present for the experimental HREM image as well, although the intensity is somewhat weaker. This is clearly seen by replotting Fig. 8 on a narrower scale of -0.005 $Å^{-1}$ to 0.005 $Å^{-1}$ (see Figs. 8(c,d) for α_{13} and α_{23} respectively). The mottled contrast due to the experimental noise precludes characterization of the extremely small in-plane displacements of a screw dislocation in bcc Mo by HREM.

The final conclusions of this study have been summarized as follows [14]:

1. The Nye tensor method was used to analyze FS, first-principles and BOP predicted ½<111> screw dislocation cores in bcc Mo. For the FS core the dislocation is split into three screw fractional dislocations with Burgers vector of approximately **b**/3. The first-principles and BOP cores, however, show a more localized structure. α_{13} and α_{23} Nye tensor plots reveal the distribution of the edge fractional dislocations. From such plots Burgers vector magnitudes of the edge fractional dislocations were determined for the first time.
2. The Nye tensor was confirmed to be 'blind' to compatible deformations such as the Eshelby twist around an end-on screw dislocation in a thin TEM foil. This is true even for two dimensional HREM images. The technique could therefore be used to remove displacements due to surface relaxation in experimental HREM micrographs.

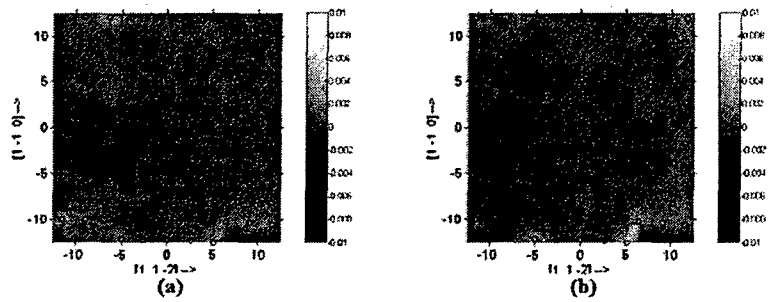


Fig. 7: α_{13} (a) and α_{23} (b) Nye tensor plots for an experimental HREM image of a screw dislocation in Mo. The origin is placed at the centre of the HREM image and coincides with the dislocation core region. The Eshelby twist has been removed to within the background noise level (Figs. 7(a,b) are plotted on a scale of -0.01 $Å^{-1}$ to 0.01 $Å^{-1}$).

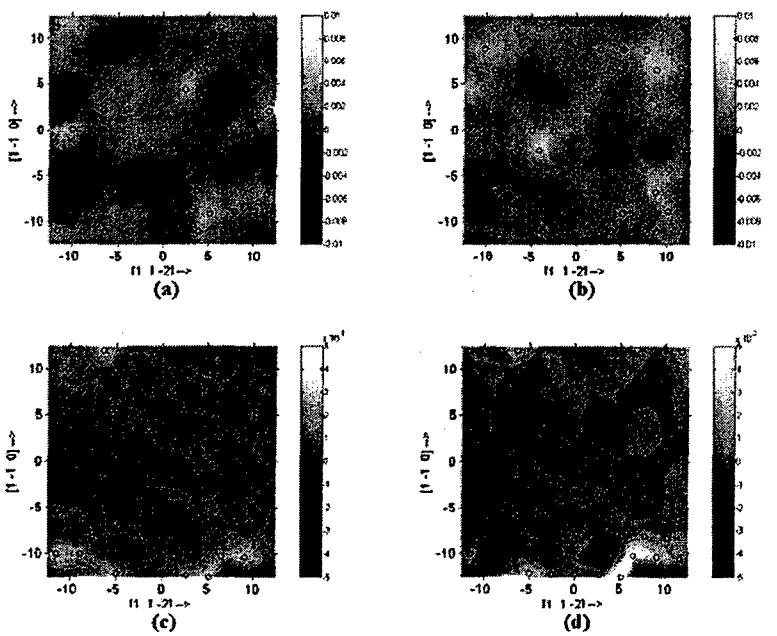


Fig. 8: α_{13} (a) and α_{23} (b) Nye tensor plots for the 2D projected, FS potential screw dislocation supercell with experimental 'noise' displacements superimposed on the atom column positions. A characteristic mottled contrast is observed due to the noise contribution. Close examination of the α_{13} and α_{23} Nye tensor plots in Fig. 7 reveals a similar contrast, which can be seen by plotting the experimental HREM image α_{13}, α_{23} plots on a scale between -0.005 $Å^{-1}$ and 0.005 $Å^{-1}$ in Figs. 8(c,d).

3. The Nye tensor plots for the experimental HREM images showed a weak, mottled contrast. This contrast is due to the experimental noise in the HREM image. The noise in an HREM image of a <111> oriented, perfect crystal region of Mo was characterized and superimposed on the 2D projected supercells of the FS, BOP and first-principles simulated screw dislocation cores. The Nye tensor plots for these modified supercells resulted in a mottled contrast, similar to the experimental results, which masked the true structure of the dislocation core. This shows that experimental noise precludes characterization of the in-plane displacements of screw dislocations in Mo by HREM.
4. The Nye tensor method is insensitive to small misalignments (e.g. ~ 2° misalignment for a 5 nm thick foil) of the TEM foil away from the ideal zone axis, i.e. no 'spurious' signals due to the in-plane component of the ½<111> Burgers vector that may be confused with the edge fractional dislocations are generated.

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V. PERSONNEL SUPPORTED

- Professor Kevin J. Hemker; PI;
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  currently a Professor at Tohoku University.

- Dr. Budhika Mendis,
  partially support as a post-doctoral fellow in years 2 and 3.

VI. PUBLICATIONS RELATED TO THIS GRANT

- Jong Lee and K.J. Hemker, Editors of "Special Issue on Defects and Deformation of Crystalline Solids", Philosophical Magazine, **85** (2005) 115-397.

- Jong Lee and K.J. Hemker, "Festschrift for Dr. Man Hyung Yoo", Philosophical Magazine, **85** (2005) 115-116.

- B.G. Mendis, Y. Mishin, C.S. Hartley, and K.J. Hemker, "HREM imaging of screw dislocation core structures in bcc metals", Material Research Society Proceedings, **839** (2005) P3.13.1-6.

- B.G. Mendis, Y. Mishin, C.S. Hartley, and K.J. Hemker, "Use of the Nye tensor in analyzing HREM images of bcc screw dislocations", Philosophical Magazine *(invited submission for special issue on the 50th anniversary of TEM observations of dislocations)*, under review.

VII. AWARDS RELATED TO THIS GRANT

No major awards at this time.

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13. SUPPLEMENTARY NOTES

14. ABSTRACT

The scientific aim of this study was to use state-of-the-art TEM techniques to experimentally describe dislocation core structures in bcc metals through experimental characterization of screw dislocations in single-crystalline Mo. Methods were developed for deriving localized electron structure data from electron energy loss spectra (EELS) taken from perfect lattice regions and along dislocations and low angle boundaries in ordered NiAl. Significant changes in the fine structure of the NiL edge were associated with <001> dislocations in NiAl and comparisons with first-principles were used to characterize localized electronic structure and bonding in the vicinity of this dislocation. However, difficulties associated with the position of the energy edges for Mo precluded application of this technique to the study of 1/2<111> screw dislocations in single-crystalline Mo. For this reason, the majority of this study focused on : direct HREM observations of the atomic columns surrounding 1/2<111> screw dislocations in Mo, characterization of the displacement fields associated with these dislocations, mitigation of experimental noise, and comparison of the experimental observations with theoretically predicted dislocation structures.

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